

Toluene  
108-88-3 | DTXSID7021360

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

## Model Results

**Predicted value:** 3.87

**Global applicability domain:** Inside

**Local applicability domain index:** 9.93e-01

**Confidence level:** 5.64e-01

## Nearest Neighbors from the Training Set

Image not found

Toluene

**Measured:** 3.31

**Predicted:** 3.87

Image not found

Hexanal

**Measured:** 4.41

**Predicted:** 3.86

Image not found

Methylcyclohexane

**Measured:** 3.03

**Predicted:** 3.59

Image not found

2-Hexanone

**Measured:** 3.68

**Predicted:** 3.66

Image not found

Dimethyl sulfoxide

**Measured:** 4.96

**Predicted:** 3.99